Aggregation of $[Ln^{III}_{12}]$ clusters by the dianion of 3-formyl-salicylic acid. Synthesis, crystal structures, magnetic and luminescence properties

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Table S1. Crystallographic data, details of data collection and structure refinement parameters for compounds **1** - **3**.

Compound	**1**	**2**	**3**
empirical formula	$C_{144}H_{172}Eu_{12}N_{16}O_{76}$	$C_{141}H_{165}Gd_{12}N_{15}O_{75}$	$C_{142.5}H_{168.5}Dy_{12}N_{15.5}O_{75.50}$
Fw	5166.50	5156.88	5256.42
T [K]	170	200	200
space group	P-1	P-1	P-1
a [Å]	17.1451(6)	17.2173(12)	17.0435(6)
b [Å]	17.1531(7)	17.2380(11)	17.1107(5)
c [Å]	17.7334(7)	17.9087(9)	17.8280(6)
α [°]	70.087(4)	71.244(5)	71.221(3)
β [°]	87.863(3)	84.760(5)	84.773(3)
γ [°]	86.218(3)	87.213(5)	87.821(3)
V [Å^3]	4892.1(3)	5016.6(5)	4901.7(3)
Z	1	1	1
ρ_{calcd} [g cm^{-3}]	1.754	1.707	1.781
μ [mm^{-1}]	3.870	3.988	4.596
Crystal size [mm]	0.50 × 0.20 × 0.15	0.35 × 0.20 × 0.05	0.30 × 0.15 × 0.02
2Θ range	3.38 to 48.82	3.24 to 46.52	3.264 to 50.054
Reflections collected	41593	33305	41006
Independent reflections	16003 [R_{int}= 0.0456]	16003 [R_{int}= 0.0883]	17250 [R_{int}= 0.0579]
Data/restraints/parameters	16003/37/1063	14368/112/1084	17250/22/1075
R_1[a]	0.0515	0.0805	0.0565
wR_2[b]	0.1452	0.2111	0.1473
GOF[c]	1.006	1.040	1.032

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.
[c] GOF = $\{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$, where n is the number of reflections and p is the total number of parameters refined.

Table S2. SHAPE analysis for the Ln^{III} ions in compounds **1-3**.

ML_8	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8
Eu1	32.219	22.921	16.356	10.705	3.769	1.232	12.531	27.685	1.848	1.573	2.630	10.864	24.064
Eu3A	31.183	22.849	15.335	9.180	2.568	0.800	14.605	28.265	2.771	2.206	2.739	9.634	23.501
Eu3B	32.382	22.549	15.578	8.858	2.290	0.881	14.331	28.233	2.884	2.593	2.975	9.297	23.332
Eu5A	29.363	24.303	16.808	9.969	1.405	1.362	13.706	27.701	2.437	2.325	3.189	10.362	24.159
Eu5B	30.264	23.230	14.247	8.303	1.337	1.681	14.835	27.576	2.740	2.300	4.040	8.659	22.096
Eu6	31.463	22.830	14.833	8.647	2.077	0.964	15.037	27.797	2.445	2.305	3.003	9.066	22.929
Gd1	31.564	22.726	14.493	8.525	2.120	0.944	14.869	27.517	2.494	2.368	2.987	8.934	22.750
Gd3	29.089	24.044	15.539	9.220	1.254	1.425	14.048	27.017	2.588	2.164	3.348	9.542	22.894
Gd5	31.958	23.190	16.430	10.456	3.723	1.122	12.761	28.053	2.018	1.649	2.593	10.646	23.861
Gd6	31.987	22.770	15.527	8.820	2.322	0.839	14.671	28.056	2.838	2.470	2.951	9.299	23.100
Dy1	30.945	23.009	15.166	8.867	1.920	0.976	14.686	27.867	2.241	2.115	2.920	9.257	23.124
Dy2	29.319	23.979	15.928	9.360	1.264	1.383	13.753	27.336	2.501	2.259	3.277	9.656	22.885
Dy5	31.671	22.652	15.709	9.088	2.318	0.827	14.251	27.888	2.772	2.448	2.811	9.519	23.123
Dy6	31.901	23.092	16.576	10.572	3.762	1.136	12.514	27.814	1.872	1.690	2.434	10.655	24.303

Table S3. Selected bond distances and angles for compound **1**, **2**, and respectively, **3**

Bond lengths (Å)		
1	**2**	**3**
Eu1-O2 = 2.496(7)	Gd1-O1 = 2.352(12)	Dy1-O1 = 2.296(6)
Eu1-O3 = 2.258(7)	Gd1-O2 = 2.421(11)	Dy1-O3 = 2.408(6)
Eu1-O6 = 2.656(7)	Gd1-O8 = 2.545(11)	Dy1-O8 = 2.512(6)
Eu1-O21 = 2.368(7)	Gd1-O9 = 2.258(11)	Dy1-O9 = 2.237(8)
Eu1-O25 = 2.412(8)	Gd1-O12 = 2.490(12)	Dy1-O11 = 2.467(7)
Eu1-O26 = 2.329(7)	Gd1-O13 = 2.256(13)	Dy1-O13 = 2.261(7)
Eu1-O33 = 2.374(6)	Gd1-O27 = 2.332(11)	Dy1-O15 = 2.322(7)
Eu1-O34 = 2.376(6)	Gd1-O31 = 2.410(12)	Dy1-O35 = 2.416(8)
Eu2-O2 = 2.506(6)	Gd2-O2 = 2.350(10)	Dy2-O1 = 2.276(6)
Eu2-O13 = 2.538(7)	Gd2-O3 = 2.384(11)	Dy2-O2 = 2.377(6)
Eu2-O14 = 2.534(6)	Gd2-O4 = 2.451(11)	Dy2-O8 = 2.612(6)
Eu2-O18 = 2.510(7)	Gd2-O5 = 2.473(11)	Dy2-O19 = 2.443(8)
Eu2-O33 = 2.408(6)	Gd2-O6 = 2.389(10)	Dy2-O21 = 2.197(7)
Eu2-O34 = 2.447(6)	Gd2-O7 = 2.556(13)	Dy2-O27 = 2.318(7)
Eu2-O35 = 2.460(6)	Gd2-O8 = 2.507(10)	Dy2-O31 = 2.320(10)
Eu2-O36 = 2.373(6)	Gd2-O20 = 2.476(11)	Dy2-O32 = 2.389(7)
Eu2-O37 = 2.360(6)	Gd2-O28 = 2.506(12)	Dy3-O1 = 2.344(7)
Eu3-O6 = 2.526(6)	Gd3-O1 = 2.310(11)	Dy3-O2 = 2.451(7)
Eu3-O7 = 2.299(7)	Gd3-O3 = 2.398(10)	Dy3-O3 = 2.420(6)
Eu3-O9 = 2.386(7)	Gd3-O8 = 2.643(11)	Dy3-O4 = 2.335(6)
Eu3-O18 = 2.499(6)	Gd3-O16 = 2.452(12)	Dy3-O5 = 2.343(6)
Eu3-O19 = 2.271(8)	Gd3-O17 = 2.220(14)	Dy3-O11 = 2.478(6)
Eu3-O33 = 2.387(7)	Gd3-O19 = 2.333(11)	Dy3-O19 = 2.478(6)
Eu3-O35 = 2.437(6)	Gd3-O32 = 2.422(12)	Dy3-O23 = 2.547(7)
Eu3-O27 = 2.417(9)	Gd3-O33 = 2.327(13)	Dy3-O24 = 2.481(7)
Eu4-O5 = 2.575(7)	Gd4-O1 = 2.359(10)	Dy4-O2 = 2.324(6)
Eu4-O6 = 2.521(6)	Gd4-O2 = 2.459(11)	Dy4-O3 = 2.323(6)
Eu4-O10 = 2.510(7)	Gd4-O3 = 2.471(9)	Dy4-O4 = 2.423(6)
Eu4-O22 = 2.497(6)	Gd4-O4 = 2.341(11)	Dy4-O5 = 2.422(6)
Eu4-O34 = 2.366(6)	Gd4-O5 = 2.354(11)	Dy4-O6 = 2.370(7)
Eu4-O35 = 2.374(6)	Gd4-O12 = 2.493(12)	Dy4-O7 = 2.538(8)
Eu4-O36 = 2.472(6)	Gd4-O16 = 2.495(12)	Dy4-O8 = 2.484(7)
Eu4-O37 = 2.446(6)	Gd4-O23 = 2.558(11)	Dy4-O16 = 2.477(6)
Eu4-O38 = 2.380(6)	Gd4-O24 = 2.526(11)	Dy4-O28 = 2.457(6)
Eu5-O1 = 2.349(6)	Gd5-O1AA = 2.325(11)	Dy5-O4 = 2.394(6)
Eu5-O10 = 2.482(7)	Gd5-O4 = 2.374(10)	Dy5-O6 = 2.358(6)
Eu5-O11 = 2.228(7)	Gd5-O6 = 2.352(10)	Dy5-O16 = 2.489(7)
Eu5-O14 = 2.631(7)	Gd5-O11 = 2.362(12)	Dy5-O17 = 2.236(7)
Eu5-O36 = 2.427(6)	Gd5-O20 = 2.463(10)	Dy5-O20 = 2.347(8)
Eu5-O38 = 2.334(6)	Gd5-O21 = 2.259(12)	Dy5-O24 = 2.487(7)
Eu5-O28 = 2.433(9)	Gd5-O24 = 2.632(11)	Dy5-O25 = 2.285(8)
Eu5-O29 = 2.362(9)	Gd5-O34 = 2.432(14)	Dy5-O36 = 2.390(10)
Eu6-O14 = 2.539(6)	Gd6-O5 = 2.425(11)	Dy6-O5 = 2.336(6)
Eu6-O15 = 2.278(7)	Gd6-O6 = 2.389(11)	Dy6-O6 = 2.332(6)
Eu6-O17 = 2.350(7)	Gd6-O15 = 2.362(12)	Dy6-O12 = 2.333(7)
Eu6-O22 = 2.494(7)	Gd6-O24 = 2.524(11)	Dy6-O24 = 2.648(6)
Eu6-O23 = 2.270(7)	Gd6-O25 = 2.291(11)	Dy6-O28 = 2.460(6)
Eu6-O30 = 2.434(7)	Gd6-O28 = 2.487(10)	Dy6-O29 = 2.221(6)
Eu6-O37 = 2.445(6)	Gd6-O29 = 2.283(13)	Dy6-O33 = 2.413(10)
Eu6-O38 = 2.337(6)	Gd6-O35 = 2.420(15)	Dy6-O34 = 2.289(8)

Angles (º)		
1	**2**	**3**
O2-Eu1-O6 = 121.2(2)	O1-Gd1-O2 = 74.3(4)	O1-Dy1-O3 = 74.2(2)
O3-Eu1-O2 = 69.8(2)	O1-Gd1-O8 = 66.2(4)	O1-Dy1-O8 = 65.6(2)
O3-Eu1-O6 = 146.0(2)	O1-Gd1-O12 = 70.4(4)	O1-Dy1-O11 = 71.1(2)
O3-Eu1-O21 = 75.8(3)	O1-Gd1-O31 = 74.2(4)	O1-Dy1-O15 = 138.2(2)
O3-Eu1-O25 = 83.8(3)	O2-Gd1-O8 = 68.4(3)	O1-Dy1-O35 = 73.8(2)
O3-Eu1-O26 = 113.1(3)	O2-Gd1-O12 = 65.0(4)	O3-Dy1-O8 = 68.3(2)
O3-Eu1-O33 = 139.6(2)	O9-Gd1-O1 = 98.1(4)	O3-Dy1-O11 = 65.2(2)
O3-Eu1-O34 = 91.2(2)	O9-Gd1-O2 = 138.2(4)	O3-Dy1-O35 = 134.9(3)
O21-Eu1-O2 = 132.8(2)	O9-Gd1-O8 = 71.0(4)	O9-Dy1-O1 = 98.7(3)
O21-Eu1-O6 = 74.9(2)	O9-Gd1-O12 = 151.9(4)	O9-Dy1-O3 = 138.9(3)
O21-Eu1-O25 = 134.5(3)	O9-Gd1-O27 = 82.9(4)	O9-Dy1-O8 = 72.0(2)
O21-Eu1-O33 = 137.6(2)	O9-Gd1-O31 = 76.1(5)	O9-Dy1-O11 = 151.8(2)
O21-Eu1-O34 = 84.0(2)	O12-Gd1-O8 = 122.6(4)	O9-Dy1-O13 = 106.3(3)
O25-Eu1-O2 = 72.6(3)	O13-Gd1-O1 = 135.4(4)	O9-Dy1-O15 = 82.0(3)
O25-Eu1-O6 = 129.6(3)	O13-Gd1-O2 = 103.7(4)	O9-Dy1-O35 = 77.1(3)
O26-Eu1-O2 = 144.8(3)	O13-Gd1-O8 = 155.9(4)	O11-Dy1-O8 = 122.8(2)
O26-Eu1-O6 = 77.2(2)	O13-Gd1-O9 = 109.3(5)	O13-Dy1-O1 = 137.2(3)
O26-Eu1-O21 = 78.5(3)	O13-Gd1-O12 = 68.9(4)	O13-Dy1-O3 = 105.3(3)
O26-Eu1-O25 = 72.9(3)	O13-Gd1-O27 = 81.1(4)	O13-Dy1-O8 = 155.4(3)
O26-Eu1-O33 = 98.4(2)	O13-Gd1-O31 = 79.0(4)	O13-Dy1-O11 = 70.5(3)
O26-Eu1-O34 = 145.0(2)	O27-Gd1-O1 = 138.2(4)	O13-Dy1-O15 = 80.2(3)
O33-Eu1-O2 = 69.9(2)	O27-Gd1-O2 = 77.6(4)	O13-Dy1-O35 = 78.7(3)
O33-Eu1-O6 = 63.4(2)	O27-Gd1-O8 = 75.0(4)	O15-Dy1-O3 = 78.2(2)
O33-Eu1-O25 = 81.9(3)	O27-Gd1-O12 = 123.1(4)	O15-Dy1-O8 = 75.3(2)
O33-Eu1-O34 = 74.8(2)	O27-Gd1-O31 = 144.1(5)	O15-Dy1-O11 = 123.4(3)
O34-Eu1-O2 = 65.9(2)	O31-Gd1-O2 = 136.2(5)	O15-Dy1-O35 = 144.6(3)
O34-Eu1-O6 = 69.1(2)	O31-Gd1-O8 = 123.0(4)	O35-Dy1-O8 = 123.2(2)
O34-Eu1-O25 = 137.2(2)	O31-Gd1-O12 = 76.1(4)	O35-Dy1-O11 = 74.9(3)
O2-Eu2-O13 = 72.3(2)	O2-Gd2-O3 = 69.1(4)	O1-Dy2-O2 = 75.5(2)
O2-Eu2-O14 = 91.7(2)	O2-Gd2-O4 = 115.8(4)	O1-Dy2-O8 = 64.2(2)
O2-Eu2-O18 = 132.6(2)	O2-Gd2-O5 = 80.6(3)	O1-Dy2-O19 = 71.5(2)
O14-Eu2-O13 = 51.7(2)	O2-Gd2-O6 = 146.3(4)	O1-Dy2-O27 = 138.0(2)
O18-Eu2-O13 = 71.6(2)	O2-Gd2-O7 = 113.4(4)	O1-Dy2-O31 = 106.9(3)
O18-Eu2-O14 = 89.4(2)	O2-Gd2-O8 = 70.1(4)	O1-Dy2-O32 = 70.8(2)
O33-Eu2-O2 = 69.2(2)	O2-Gd2-O20 = 145.3(4)	O2-Dy2-O8 = 68.5(2)
O33-Eu2-O13 = 69.9(2)	O2-Gd2-O28 = 79.1(4)	O2-Dy2-O19 = 66.1(2)
O33-Eu2-O14 = 121.5(2)	O3-Gd2-O4 = 80.3(4)	O2-Dy2-O32 = 135.3(3)
O33-Eu2-O18 = 70.3(2)	O3-Gd2-O5 = 117.0(4)	O19-Dy2-O8 = 122.4(2)
O33-Eu2-O34 = 73.0(2)	O3-Gd2-O6 = 142.9(3)	O21-Dy2-O1 = 138.2(3)
O34-Eu2-O2 = 64.7(2)	O3-Gd2-O7 = 112.9(4)	O21-Dy2-O2 = 107.7(3)
O34-Eu2-O13 = 130.6(2)	O3-Gd2-O8 = 72.1(4)	O21-Dy2-O8 = 157.0(3)
O34-Eu2-O14 = 147.1(2)	O3-Gd2-O20 = 77.2(3)	O21-Dy2-O19 = 72.4(3)
O34-Eu2-O18 = 123.4(2)	O3-Gd2-O28 = 147.1(3)	O21-Dy2-O27 = 81.0(3)
O34-Eu2-O35 = 65.9(2)	O4-Gd2-O5 = 65.1(4)	O21-Dy2-O31 = 93.3(3)
O35-Eu2-O2 = 124.8(2)	O4-Gd2-O7 = 130.5(4)	O21-Dy2-O32 = 80.8(3)
O35-Eu2-O13 = 129.7(2)	O4-Gd2-O8 = 147.4(4)	O27-Dy2-O2 = 78.2(2)
O35-Eu2-O14 = 143.2(2)	O4-Gd2-O20 = 64.8(4)	O27-Dy2-O8 = 76.0(2)
O35-Eu2-O18 = 63.6(2)	O4-Gd2-O28 = 122.9(3)	O27-Dy2-O19 = 125.0(3)
O36-Eu2-O2 = 76.9(2)	O5-Gd2-O7 = 129.8(4)	O27-Dy2-O31 = 78.3(3)
O36-Eu2-O13 = 113.0(2)	O5-Gd2-O8 = 143.8(3)	O27-Dy2-O32 = 145.7(3)
O36-Eu2-O14 = 71.9(2)	O5-Gd2-O20 = 123.8(3)	O31-Dy2-O2 = 145.4(3)

O36-Eu2-O18 = 146.5(2)
O36-Eu2-O33 = 143.3(2)
O36-Eu2-O34 = 80.3(2)
O36-Eu2-O35 = 117.0(2)
O37-Eu2-O2 = 144.6(2)
O37-Eu2-O13 = 113.3(2)
O37-Eu2-O14 = 70.1(2)
O37-Eu2-O18 = 78.9(2)
O37-Eu2-O33 = 146.2(2)
O37-Eu2-O34 = 115.8(2)
O37-Eu2-O35 = 80.1(2)
O37-Eu2-O36 = 68.8(2)
O7-Eu3-O6 = 70.8(2)
O7-Eu3-O9 = 80.8(3)
O7-Eu3-O18 = 152.7(3)
O7-Eu3-O33 = 98.1(2)
O7-Eu3-O35 = 138.7(2)
O7-Eu3-O27 = 77.4(5)
O9-Eu3-O6 = 75.6(2)
O9-Eu3-O18 = 124.3(2)
O9-Eu3-O33 = 138.5(2)
O9-Eu3-O35 = 79.0(2)
O9-Eu3-O27 = 144.3(5)
O18-Eu3-O6 = 122.1(2)
O19-Eu3-O6 = 152.5(3)
O19-Eu3-O7 = 110.0(3)
O19-Eu3-O9 = 77.5(3)
O19-Eu3-O18 = 70.4(2)
O19-Eu3-O33 = 138.5(3)
O19-Eu3-O35 = 100.2(3)
O19-Eu3-O27 = 83.9(4)
O33-Eu3-O6 = 65.3(2)
O33-Eu3-O18 = 70.8(2)
O33-Eu3-O35 = 75.1(2)
O33-Eu3-O27 = 72.9(4)
O35-Eu3-O6 = 69.5(2)
O35-Eu3-O18 = 64.1(2)
O27-Eu3-O6 = 121.9(4)
O27-Eu3-O18 = 75.6(5)
O27-Eu3-O35 = 134.7(5)
O6-Eu4-O5 = 51.1(2)
O10-Eu4-O5 = 72.6(2)
O10-Eu4-O6 = 90.0(2)
O22-Eu4-O5 = 71.2(2)
O22-Eu4-O6 = 91.1(2)
O22-Eu4-O10 = 132.0(2)
O34-Eu4-O5 = 112.3(2)
O34-Eu4-O6 = 71.6(2)
O34-Eu4-O10 = 146.3(2)
O34-Eu4-O22 = 77.8(2)
O34-Eu4-O35 = 68.6(2)
O34-Eu4-O36 = 116.1(2)
O34-Eu4-O37 = 79.8(2)
O34-Eu4-O38 = 144.3(2)
O35-Eu4-O5 = 113.3(2)
O35-Eu4-O6 = 70.5(2)
O5-Gd2-O28 = 63.9(4)
O6-Gd2-O4 = 72.8(4)
O6-Gd2-O5 = 73.9(4)
O6-Gd2-O7 = 69.8(4)
O6-Gd2-O8 = 121.5(4)
O6-Gd2-O20 = 68.5(3)
O6-Gd2-O28 = 70.0(3)
O8-Gd2-O7 = 51.7(3)
O20-Gd2-O7 = 71.9(4)
O20-Gd2-O8 = 92.0(3)
O20-Gd2-O28 = 131.8(4)
O28-Gd2-O7 = 71.7(4)
O28-Gd2-O8 = 89.4(3)
O1-Gd3-O3 = 75.6(3)
O1-Gd3-O8 = 65.1(4)
O1-Gd3-O16 = 70.3(4)
O1-Gd3-O19 = 138.9(4)
O1-Gd3-O32 = 70.1(4)
O1-Gd3-O33 = 108.3(5)
O3-Gd3-O8 = 69.5(4)
O3-Gd3-O16 = 65.5(4)
O3-Gd3-O32 = 134.6(4)
O16-Gd3-O8 = 122.3(4)
O17-Gd3-O1 = 135.7(4)
O17-Gd3-O3 = 107.2(4)
O17-Gd3-O8 = 158.7(4)
O17-Gd3-O16 = 71.3(4)
O17-Gd3-O19 = 82.5(5)
O17-Gd3-O32 = 79.4(5)
O17-Gd3-O33 = 93.2(5)
O19-Gd3-O3 = 78.4(4)
O19-Gd3-O8 = 76.2(4)
O19-Gd3-O16 = 125.1(4)
O19-Gd3-O32 = 146.0(4)
O32-Gd3-O8 = 118.4(4)
O32-Gd3-O16 = 75.3(4)
O33-Gd3-O3 = 146.1(4)
O33-Gd3-O8 = 81.6(4)
O33-Gd3-O16 = 148.3(4)
O33-Gd3-O19 = 77.9(5)
O33-Gd3-O32 = 74.7(5)
O1-Gd4-O2 = 73.4(4)
O1-Gd4-O3 = 73.4(4)
O1-Gd4-O12 = 70.2(4)
O1-Gd4-O16 = 68.8(4)
O1-Gd4-O23 = 70.7(4)
O1-Gd4-O24 = 121.8(3)
O2-Gd4-O3 = 66.0(4)
O2-Gd4-O12 = 64.4(3)
O2-Gd4-O16 = 123.4(4)
O2-Gd4-O23 = 130.4(4)
O2-Gd4-O24 = 146.1(4)
O3-Gd4-O12 = 124.6(4)
O3-Gd4-O16 = 63.7(3)
O3-Gd4-O23 = 130.6(4)
O3-Gd4-O24 = 144.2(4)
O31-Dy2-O8 = 81.3(3)
O31-Dy2-O19 = 148.2(3)
O31-Dy2-O32 = 74.0(3)
O32-Dy2-O8 = 118.5(2)
O32-Dy2-O19 = 75.8(3)
O1-Dy3-O2 = 72.8(2)
O1-Dy3-O3 = 73.2(2)
O1-Dy3-O11 = 70.2(2)
O1-Dy3-O19 = 69.7(2)
O1-Dy3-O23 = 70.5(3)
O1-Dy3-O24 = 122.0(2)
O2-Dy3-O11 = 124.3(2)
O2-Dy3-O19 = 64.5(2)
O2-Dy3-O23 = 130.6(2)
O2-Dy3-O24 = 144.3(2)
O3-Dy3-O2 = 65.6(2)
O3-Dy3-O11 = 64.8(2)
O3-Dy3-O19 = 124.2(2)
O3-Dy3-O23 = 129.8(2)
O3-Dy3-O24 = 146.6(2)
O4-Dy3-O1 = 145.0(2)
O4-Dy3-O2 = 81.0(2)
O4-Dy3-O3 = 116.5(2)
O4-Dy3-O5 = 68.7(2)
O4-Dy3-O11 = 144.8(2)
O4-Dy3-O19 = 78.3(2)
O4-Dy3-O23 = 113.2(2)
O4-Dy3-O24 = 69.9(2)
O5-Dy3-O1 = 144.4(2)
O5-Dy3-O2 = 116.5(2)
O5-Dy3-O3 = 80.0(2)
O5-Dy3-O11 = 77.5(2)
O5-Dy3-O19 = 145.9(2)
O5-Dy3-O23 = 112.7(2)
O5-Dy3-O24 = 72.0(2)
O11-Dy3-O19 = 132.4(2)
O11-Dy3-O23 = 70.9(2)
O11-Dy3-O24 = 91.1(2)
O19-Dy3-O23 = 72.4(2)
O19-Dy3-O24 = 89.1(2)
O24-Dy3-O23 = 51.5(2)
O2-Dy4-O4 = 117.6(2)
O2-Dy4-O5 = 80.2(2)
O2-Dy4-O6 = 143.1(2)
O2-Dy4-O7 = 112.6(2)
O2-Dy4-O8 = 71.6(2)
O2-Dy4-O16 = 146.5(2)
O2-Dy4-O28 = 76.1(2)
O3-Dy4-O2 = 69.1(2)
O3-Dy4-O4 = 80.7(2)
O3-Dy4-O5 = 116.2(2)
O3-Dy4-O6 = 146.3(2)
O3-Dy4-O7 = 113.8(2)
O3-Dy4-O8 = 70.1(2)
O3-Dy4-O16 = 78.9(2)
O3-Dy4-O28 = 144.1(2)

O35-Eu4-O10 = 78.8(2)
O35-Eu4-O22 = 145.3(2)
O35-Eu4-O36 = 80.0(2)
O35-Eu4-O37 = 115.7(2)
O35-Eu4-O38 = 145.1(2)
O36-Eu4-O5 = 131.2(2)
O36-Eu4-O6 = 144.2(2)
O36-Eu4-O10 = 64.2(2)
O36-Eu4-O22 = 124.5(2)
O37-Eu4-O5 = 130.5(2)
O37-Eu4-O6 = 146.0(2)
O37-Eu4-O10 = 123.8(2)
O37-Eu4-O22 = 64.7(2)
O37-Eu4-O36 = 65.9(2)
O38-Eu4-O5 = 70.9(2)
O38-Eu4-O6 = 122.0(2)
O38-Eu4-O10 = 69.4(2)
O38-Eu4-O22 = 69.6(2)
O38-Eu4-O36 = 73.6(2)
O38-Eu4-O37 = 73.5(2)
O1-Eu5-O10 = 124.3(2)
O1-Eu5-O14 = 76.8(2)
O1-Eu5-O36 = 78.1(2)
O1-Eu5-O28 = 149.1(5)
O1-Eu5-O29 = 81.8(6)
O10-Eu5-O14 = 121.9(2)
O11-Eu5-O1 = 82.0(3)
O11-Eu5-O10 = 70.9(3)
O11-Eu5-O14 = 158.9(2)
O11-Eu5-O36 = 106.4(3)
O11-Eu5-O38 = 136.1(3)
O11-Eu5-O28 = 78.3(5)
O11-Eu5-O29 = 95.1(6)
O36-Eu5-O10 = 65.2(2)
O36-Eu5-O14 = 69.4(2)
O36-Eu5-O28 = 130.4(5)
O38-Eu5-O1 = 138.4(2)
O38-Eu5-O10 = 70.6(2)
O38-Eu5-O14 = 64.2(2)
O38-Eu5-O36 = 75.2(2)
O38-Eu5-O28 = 69.6(5)
O38-Eu5-O29 = 105.4(6)
O28-Eu5-O10 = 70.7(5)
O28-Eu5-O14 = 120.7(5)
O29-Eu5-O10 = 146.2(6)
O29-Eu5-O14 = 81.9(6)
O29-Eu5-O36 = 147.9(6)
O29-Eu5-O28 = 76.5(7)
O15-Eu6-O14 = 71.1(2)
O15-Eu6-O17 = 82.8(3)
O15-Eu6-O22 = 152.0(2)
O15-Eu6-O30 = 77.2(3)
O15-Eu6-O37 = 138.5(2)
O15-Eu6-O38 = 98.4(2)
O17-Eu6-O14 = 75.8(2)
O17-Eu6-O22 = 122.9(2)
O4-Gd4-O1 = 145.0(4)
O4-Gd4-O2 = 80.5(4)
O4-Gd4-O3 = 116.7(3)
O4-Gd4-O5 = 68.8(4)
O4-Gd4-O12 = 77.6(4)
O4-Gd4-O16 = 146.3(4)
O4-Gd4-O23 = 112.3(4)
O4-Gd4-O24 = 71.2(4)
O5-Gd4-O1 = 144.7(4)
O5-Gd4-O2 = 116.9(4)
O5-Gd4-O3 = 80.5(4)
O5-Gd4-O12 = 145.1(4)
O5-Gd4-O16 = 78.6(4)
O5-Gd4-O23 = 112.2(4)
O5-Gd4-O24 = 69.9(3)
O12-Gd4-O16 = 132.1(4)
O12-Gd4-O23 = 71.9(4)
O12-Gd4-O24 = 91.0(4)
O16-Gd4-O23 = 72.2(4)
O16-Gd4-O24 = 90.3(4)
O24-Gd4-O23 = 51.2(4)
O1AA-Gd5-O4 = 144.7(4)
O1AA-Gd5-O6 = 98.2(4)
O1AA-Gd5-O11 = 79.4(4)
O1AA-Gd5-O20 = 144.6(4)
O1AA-Gd5-O24 = 77.1(4)
O1AA-Gd5-O34 = 72.5(4)
O4-Gd5-O20 = 66.1(4)
O4-Gd5-O24 = 68.8(3)
O4-Gd5-O34 = 137.4(4)
O6-Gd5-O4 = 74.9(4)
O6-Gd5-O11 = 137.9(4)
O6-Gd5-O20 = 69.3(4)
O6-Gd5-O24 = 63.7(4)
O6-Gd5-O34 = 80.8(5)
O11-Gd5-O4 = 83.3(4)
O11-Gd5-O20 = 132.5(4)
O11-Gd5-O24 = 75.0(4)
O11-Gd5-O34 = 135.5(4)
O20-Gd5-O24 = 121.0(3)
O21-Gd5-O1AA = 111.7(4)
O21-Gd5-O4 = 93.3(4)
O21-Gd5-O6 = 139.7(4)
O21-Gd5-O11 = 76.0(5)
O21-Gd5-O20 = 70.7(4)
O21-Gd5-O24 = 147.3(4)
O21-Gd5-O34 = 83.2(5)
O34-Gd5-O20 = 72.8(4)
O34-Gd5-O24 = 128.7(5)
O5-Gd6-O24 = 68.8(3)
O5-Gd6-O28 = 64.9(4)
O6-Gd6-O5 = 74.8(4)
O6-Gd6-O24 = 65.0(4)
O6-Gd6-O28 = 70.4(3)
O6-Gd6-O35 = 74.7(4)
O15-Gd6-O5 = 78.0(4)
O4-Dy4-O7 = 129.6(2)
O4-Dy4-O8 = 143.9(2)
O4-Dy4-O16 = 64.6(2)
O4-Dy4-O28 = 124.7(2)
O5-Dy4-O4 = 66.00(19)
O5-Dy4-O7 = 129.6(2)
O5-Dy4-O8 = 146.6(2)
O5-Dy4-O16 = 124.5(2)
O5-Dy4-O28 = 64.5(2)
O6-Dy4-O4 = 74.1(2)
O6-Dy4-O5 = 73.2(2)
O6-Dy4-O7 = 69.1(3)
O6-Dy4-O8 = 121.2(3)
O6-Dy4-O16 = 70.3(2)
O6-Dy4-O28 = 69.6(2)
O8-Dy4-O7 = 52.1(2)
O16-Dy4-O7 = 71.3(2)
O16-Dy4-O8 = 88.7(2)
O28-Dy4-O7 = 71.7(2)
O28-Dy4-O8 = 91.1(2)
O28-Dy4-O16 = 132.7(2)
O4-Dy5-O16 = 64.8(2)
O4-Dy5-O24 = 68.8(2)
O6-Dy5-O4 = 74.8(2)
O6-Dy5-O16 = 70.3(2)
O6-Dy5-O24 = 65.9(2)
O6-Dy5-O36 = 74.2(3)
O17-Dy5-O4 = 101.1(3)
O17-Dy5-O6 = 139.2(3)
O17-Dy5-O16 = 71.4(2)
O17-Dy5-O20 = 76.2(3)
O17-Dy5-O24 = 151.4(3)
O17-Dy5-O25 = 109.2(3)
O17-Dy5-O36 = 82.0(3)
O20-Dy5-O4 = 79.7(2)
O20-Dy5-O6 = 139.5(2)
O20-Dy5-O16 = 125.0(3)
O20-Dy5-O24 = 75.7(2)
O20-Dy5-O36 = 142.8(3)
O24-Dy5-O16 = 122.3(2)
O25-Dy5-O4 = 138.7(2)
O25-Dy5-O6 = 98.0(2)
O25-Dy5-O16 = 151.6(3)
O25-Dy5-O20 = 81.0(3)
O25-Dy5-O24 = 71.2(2)
O25-Dy5-O36 = 78.2(3)
O36-Dy5-O4 = 134.5(3)
O36-Dy5-O16 = 73.7(3)
O36-Dy5-O24 = 124.6(3)
O5-Dy6-O24 = 69.1(2)
O5-Dy6-O28 = 65.7(2)
O5-Dy6-O33 = 138.0(3)
O6-Dy6-O5 = 75.5(2)
O6-Dy6-O12 = 137.5(2)
O6-Dy6-O24 = 63.6(2)
O6-Dy6-O28 = 70.2(2)

O17-Eu6-O30 = 144.6(3)	O15-Gd6-O6 = 138.3(4)	O6-Dy6-O33 = 81.7(3)
O17-Eu6-O37 = 77.8(2)	O15-Gd6-O24 = 75.9(4)	O12-Dy6-O5 = 83.9(2)
O22-Eu6-O14 = 122.3(2)	O15-Gd6-O28 = 124.0(4)	O12-Dy6-O24 = 74.4(2)
O23-Eu6-O14 = 156.1(2)	O15-Gd6-O35 = 143.9(4)	O12-Dy6-O28 = 132.9(2)
O23-Eu6-O15 = 108.6(3)	O25-Gd6-O5 = 138.0(4)	O12-Dy6-O33 = 134.2(3)
O23-Eu6-O17 = 80.4(3)	O25-Gd6-O6 = 98.5(4)	O28-Dy6-O24 = 121.2(2)
O23-Eu6-O22 = 69.5(2)	O25-Gd6-O15 = 81.3(4)	O29-Dy6-O5 = 93.3(3)
O23-Eu6-O30 = 78.8(3)	O25-Gd6-O24 = 70.9(4)	O29-Dy6-O6 = 141.2(2)
O23-Eu6-O37 = 103.9(3)	O25-Gd6-O28 = 152.6(4)	O29-Dy6-O12 = 75.7(3)
O23-Eu6-O38 = 135.9(2)	O25-Gd6-O35 = 78.7(4)	O29-Dy6-O24 = 146.6(3)
O30-Eu6-O14 = 123.0(2)	O28-Gd6-O24 = 121.8(4)	O29-Dy6-O28 = 71.4(2)
O30-Eu6-O22 = 75.1(2)	O29-Gd6-O5 = 100.3(4)	O29-Dy6-O33 = 82.7(3)
O30-Eu6-O37 = 135.1(2)	O29-Gd6-O6 = 138.1(4)	O29-Dy6-O34 = 111.1(3)
O37-Eu6-O14 = 68.7(2)	O29-Gd6-O15 = 77.5(4)	O33-Dy6-O24 = 129.4(3)
O37-Eu6-O22 = 64.8(2)	O29-Gd6-O24 = 152.9(5)	O33-Dy6-O28 = 73.6(3)
O38-Eu6-O14 = 65.7(2)	O29-Gd6-O25 = 110.4(4)	O34-Dy6-O5 = 144.9(2)
O38-Eu6-O17 = 138.4(2)	O29-Gd6-O28 = 70.1(4)	O34-Dy6-O6 = 97.6(2)
O38-Eu6-O22 = 70.3(2)	O29-Gd6-O35 = 81.8(5)	O34-Dy6-O12 = 78.6(3)
O38-Eu6-O30 = 73.9(2)	O35-Gd6-O5 = 135.1(4)	O34-Dy6-O24 = 77.0(2)
O38-Eu6-O37 = 74.2(2)	O35-Gd6-O24 = 123.8(4)	O34-Dy6-O28 = 145.0(3)
	O35-Gd6-O28 = 74.3(4)	O34-Dy6-O33 = 72.2(3)

Table S4. Parameters obtained by fitting the Cole-Cole plots using the modified Debye model.

T / K	χ_S	χ_T	τ /s	α
1.90E+00	1.037E+01	6.144E+01	1.67E-04	3.32E-01
2.10E+00	1.012E+01	5.616E+01	1.59E-04	3.05E-01
2.30E+00	9.741E+00	5.247E+01	1.49E-04	2.90E-01
2.50E+00	8.461E+00	4.835E+01	1.32E-04	2.94E-01
2.70E+00	8.663E+00	4.546E+01	1.38E-04	2.76E-01
2.90E+00	8.255E+00	4.207E+01	1.31E-04	2.59E-01
3.10E+00	9.008E+00	3.974E+01	1.33E-04	2.26E-01
3.30E+00	7.567E+00	3.765E+01	1.24E-04	2.49E-01
3.50E+00	7.487E+00	3.540E+01	1.23E-04	2.36E-01
3.70E+00	6.046E+00	3.344E+01	1.09E-04	2.43E-01
3.90E+00	6.877E+00	3.230E+01	1.16E-04	2.26E-01
4.10E+00	7.816E+00	3.097E+01	1.20E-04	2.12E-01
4.30E+00	7.423E+00	2.975E+01	1.18E-04	2.14E-01
4.50E+00	5.612E+00	2.863E+01	1.01E-04	2.26E-01
4.70E+00	5.737E+00	2.747E+01	1.01E-04	2.14E-01
4.90E+00	5.497E+00	2.643E+01	9.75E-05	2.14E-01
5.10E+00	5.133E+00	2.548E+01	9.26E-05	2.14E-01
5.30E+00	5.480E+00	2.459E+01	9.28E-05	2.07E-01
5.50E+00	6.978E+00	2.376E+01	9.84E-05	2.01E-01
5.70E+00	6.830E+00	2.299E+01	9.49E-05	2.03E-01
5.90E+00	7.427E+00	2.222E+01	1.01E-04	1.88E-01
6.10E+00	6.112E+00	2.152E+01	8.14E-05	2.00E-01
6.30E+00	5.862E+00	2.090E+01	7.52E-05	2.01E-01
6.50E+00	6.945E+00	2.031E+01	8.08E-05	1.95E-01
6.70E+00	6.034E+00	1.975E+01	6.73E-05	2.01E-01
6.90E+00	5.620E+00	1.919E+01	5.90E-05	2.12E-01
7.10E+00	6.142E+00	1.868E+01	5.73E-05	2.05E-01
7.30E+00	5.267E+00	1.823E+01	4.84E-05	2.09E-01
7.50E+00	5.174E+00	1.777E+01	4.33E-05	2.12E-01
7.70E+00	5.645E+00	1.737E+01	4.00E-05	2.24E-01
7.90E+00	6.653E+00	1.694E+01	4.22E-05	2.27E-01
8.10E+00	4.918E+00	1.650E+01	3.05E-05	2.23E-01
8.30E+00	5.093E+00	1.615E+01	2.79E-05	2.23E-01
8.50E+00	7.961E+00	1.581E+01	3.93E-05	2.08E-01

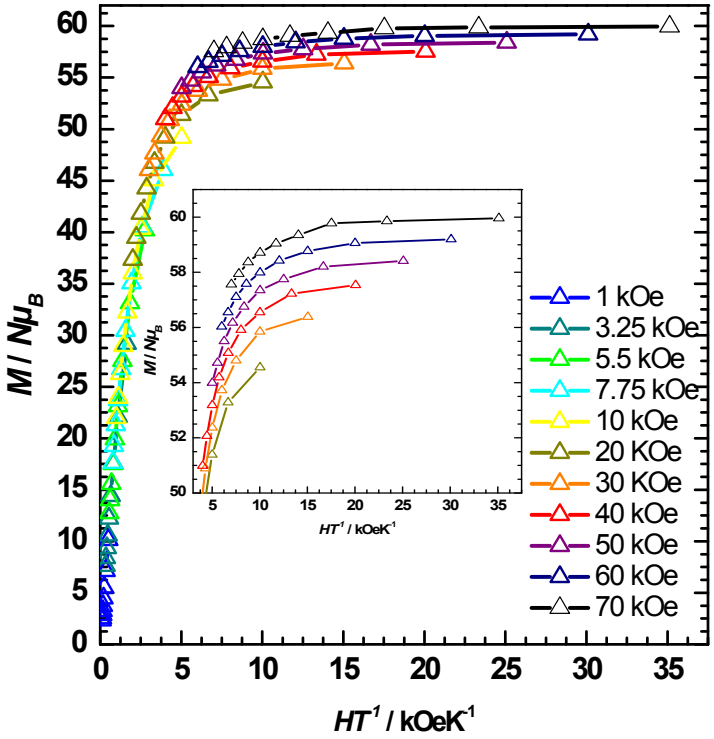

Figure S1. Reduced magnetization in M vs HT^{-1} H for **3**. Solid lines are guides for the eyes.